Paradoxes of turbulent premixed combustion and a paradigm of RANS and LES modeling

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We analyze a paradigm (basic principles), which explains discussed below paradoxial properties of turbulent premixed flames and practically resolves on a self-empirical level two main fundamental difficulties of turbulent premixed combustion modelling. These difficulties are the following:

1. Controlling combustion rate small-scale coupling of turbulence and chemistry, which cannot be resolve in the context of RANS and LES tools (so-called “challenge of turbulent combustion”). It means strictly speaking that combustion rates can be predicted directly only in context of DNS.
2. A counter-gradient scalar transport phenomenon, which makes questionable using traditional turbulence model in the flame especially for prediction of the scalar fluxes (species and temperature).

The paradigm is based on two assumptions:

1. Statistical equilibrium of small-scale structures of reaction zones: thin and in general case micro-turbulent flamelet and small-scale sheet wrinkles. It permits to express the flamelet speed and width, mean sheet area (controlling mainly by the small-scale wrinkles) and hence the flame speed in terms of resolved large scale turbulent parameters and the chemical time [1], [2]. In fact, it is a generalized for combustion known Kolmogorov’s paradigm [3], [4], which is one of the cornerstones of turbulence modelling.
2. A gasdynamic (not turbulent) nature of the counter-gradient scalar flux, which is caused by different acceleration of heavy reactant and light product by the pressure gradient generated by combustion. So traditional turbulence models with gradient approximations are applicable (at least as a first approximation) for estimation of turbulent components of the mean scalar flux while a gasdynamics estimation of the conditional average speeds of reactant and product results in the pressure-driven counter-gradient component of the flux [5], [6]. Balance between them is responsible for transition from the gradient to counter-gradient direction of scalar fluxes observed along turbulent flames.

This paradigm explains paradoxical properties of the turbulent premixed flame qualitatively and substantially quantitatively, it is a cornerstone of our model

Paradoxes of turbulent premixed combustion

Paradox 1: In experiments the width of the micro-turbulent flamelet δ_f is thin: $\delta_f / \delta_L \approx 3-5$ and (at weaker turbulence) $\delta_f / \delta_L \approx 0.5$, i.e. even less than δ_L !

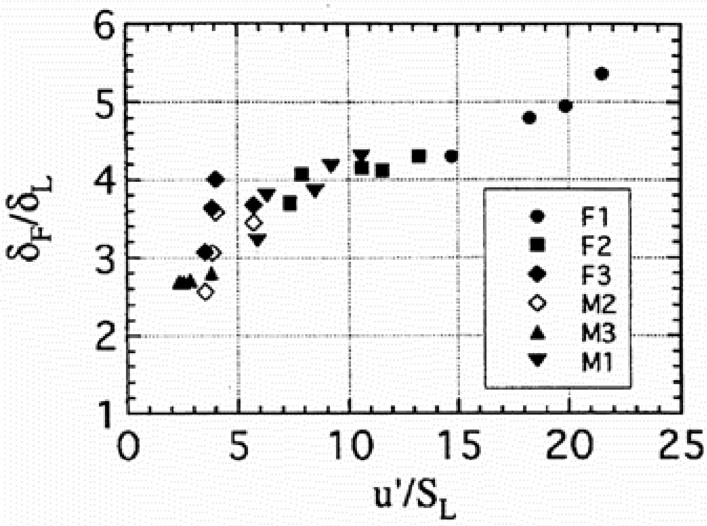


Fig. 5. Mean flamelet width for different flames from [25] **Chen, Mansour (1998) [7]**

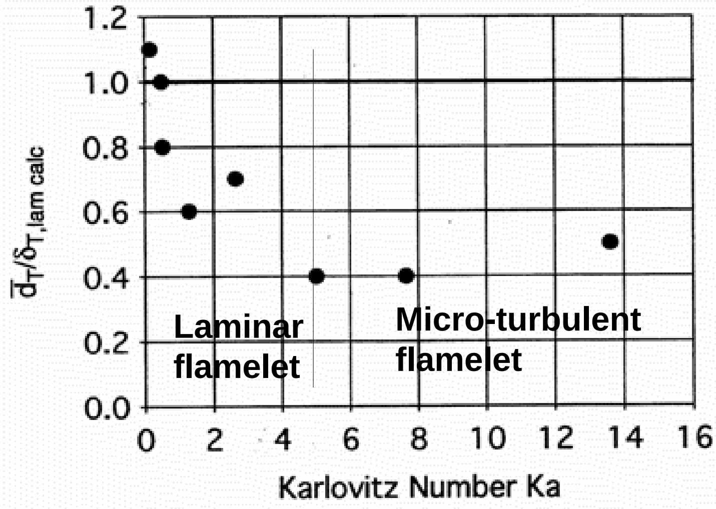


Fig. 3. The flamelet width in the turbulent flame from [22] **Dinkelacker *et al* (1996) [8]**

Question:

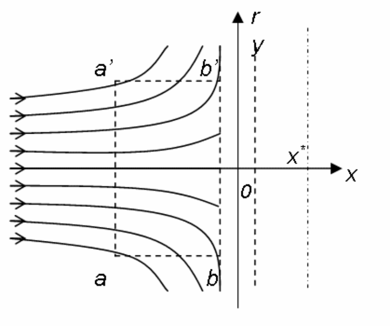
Why micro-turbulent flamelet remains thin in spite of continuous spectrum of eddies in developed turbulence, i.e. why there is no consecutive involving larger eddies in the thickened flamelet till formation distributed combustion?

Explanation:

1.The flamelet width is controlled by the chemical time and a micro-turbulent diffusion coefficient, which depends on the flamelet width $D_f \approx \varepsilon^{1/3}\delta_f^{4/3}$. In the normal (non-stretched) flamelet the micriturbulent flux, chemical release and flow convection are of the same order of magnitude and it is a physical reason of the limit of the flamelet broadening. Parameters of the flamelet are [1], [2]:

$$U_f \approx (\varepsilon\tau_{ch})^{1/2} \approx u' \cdot Da^{-1/2}, \quad \delta_f \approx \varepsilon^{1/2}\tau_{ch}^{3/2} \approx L \cdot Da^{-3/2}, \quad D_f \approx D_t \cdot Da^{-2}$$

2. External turbulence stretches the thickened flamelet and reduces U_f and δ_f. Estimations following to Karlovitz (1953) and Klimov (1963) analysis (see [9]) results in that if outer turbulence is also 5/3 inertial and it controlled by the dissipation rate we must expect two times decreasing of U_f and δ_f. Moreover, assuming for $\eta = \delta_L$ that outer turbulence is inertial, in this case estimation gives also two times reduction of the laminar flamelet due to stretch-effect. We hope that these estimations are useful for explanation.



. 2 Flamelet in a diverging flow of fuel mixture

Paradox 2: Premixed flames is characterized by increasing width and nearly constant inclination (i.e. nearly constant turbulent combustion speed U_t).

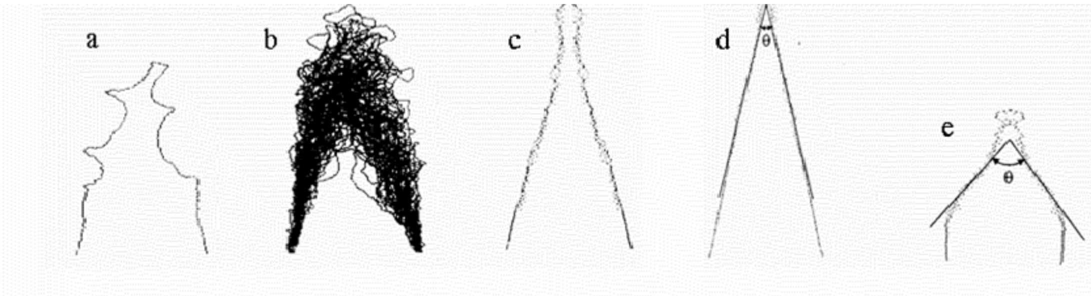
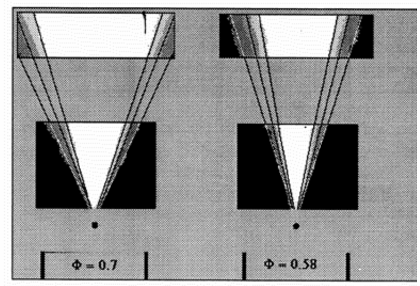
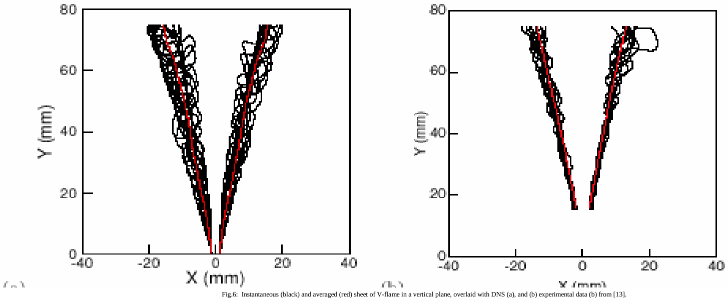


Fig.9 Instantaneous images of the flamelet sheet (a,b) and its mathematical expectation (c)-(e)[
The Bunsen flame at high pressure (Kobayashi, Tamura, Maruta, Niioka, Williams, 1996 [10])





DNS (left) and experiment (right)
(**J.B. Bell, M.S. Day, I.G. Shepherd, R. Cheng, 2003 [12]**)

Fig.7 Experimental mean reaction progress variable c(x,y) in the plane perpendicular to the flame holder for different stoichiometric ratios [33]. Fitted contour lines $\bar{c}$=0.1, 0.5, 0.9. **(V-flame. Dinkelacker, Holzler ,2000 [11])**

Question:
Why increasing of the flame width is not accompanied by corresponding increasing of the flame speed in contrast to the property of the laminar flame?

Explanation:
The turbulent flame speed is proportional to the sheet area, which is controlled mainly by small-scale wrinkles, while the brush width is controlled mainly by large-scale wrinkles. In real flames the small-scale wrinkles are statistically quasi-equilibrium while the large-scale wrinkles are not.

Estimations in [1], [2] result in the following:

$U_t = U_f(\bar{A}/A_0)$ `- expression for the flame speed

$z = h(x,y,t)$ - equation of the random flamelet sheet

$$(\bar{A}/A_0) = \overline{(1+|\nabla h|^2)^{1/2}} \approx \overline{|\nabla h|} \approx \left(\overline{|\nabla h|^2}\right)^{1/2} = \left(\int_0^\infty k^2 F(k)dk\right)^{1/2}$$

$$\delta_f \approx (\sigma_f^2)^{1/2} = \left(\int_0^\infty F(k)dk\right)^{1/2}$$

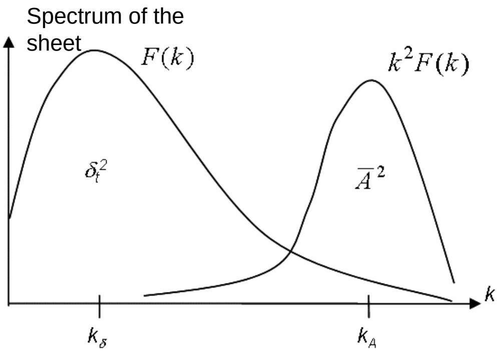
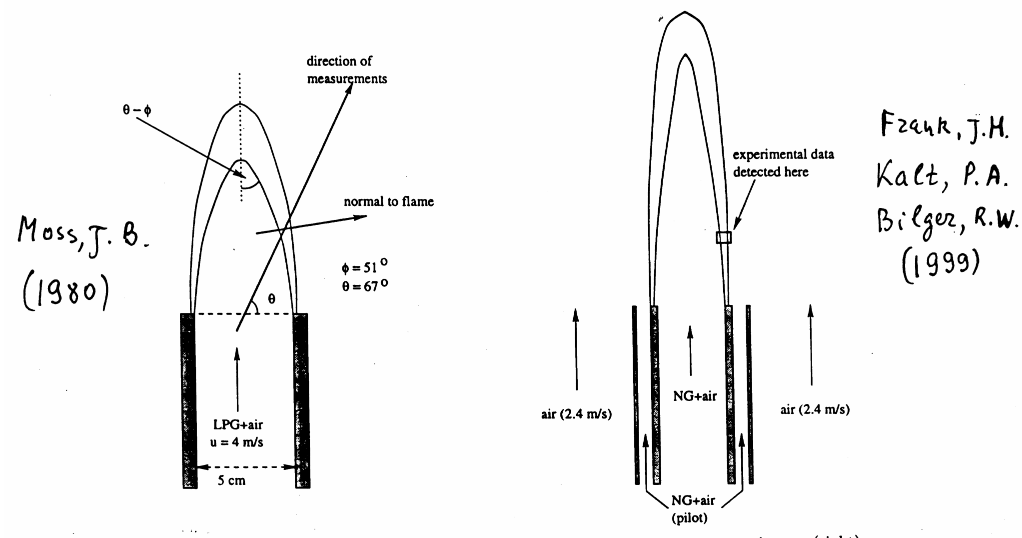


Fig.11 Spectral contributions in δ_t and $\bar{A}$

Paradox 3: Observed turbulent premixed flames have increasing brush not only at gradient, but also at neutral and counter-gradient scalar transport.



Schematics of combustor in Moss (1978) experiments (left) and Frank *et al.* (1999) experiments (right).

Question: Why the flame width increases at negative diffusion?

Explanation: The counter-gradient transport is not turbulent but a gasdynamic phenomenon so there are two different mechanisms, controlling the scalar flux:
1. Random turbulent pulsation of the speed results in gradient component;
2. Gasdynamic different acceleration of reactant and product gives the counter-gradient component, " the counter-gradient turbulent diffusion" is a misnomer.

$$\overline{\rho\vec{u}''c''} = \tilde{c}(1-\tilde{c})(\overline{\vec{u}}_b - \overline{\vec{u}}_u) = \tilde{c}(1-\tilde{c})(\Delta\overline{\vec{u}}_{turb} + \Delta\overline{\vec{u}}_{gasdyn}) \qquad \overline{\rho\vec{u}''c''}_{turb} = -\overline{\rho}D_t\nabla\tilde{c}$$

$\Delta\overline{\vec{u}}_{gasdyn}$ is calculated assuming that the total pressure of reactant is constant.

If (as a first approximation) we ignore interaction between this mechanisms, we can estimate the turbulent diffusion coefficient using standard turbulence model and
use it for modeling increasing width of the flame.

Comparison of calculations (V. Zimont, F. Biagioli, 2002 [5]) with experiments:

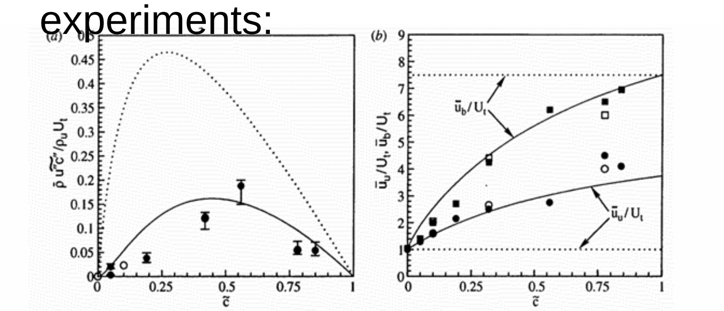


Fig.13 Comparison of (a) progress variable flux and (b) conditional velocities from Moss experiment. Simulations: (····) results from upper estimation of $\overline{\rho u''c''}$, (——) results from the gasdynamic model. Experiments: (a) (•) calculated in [42] from Moss measured conditional mean velocities, (o) calculated in [42] from Moss measured $\overline{\rho u''c''}$, (b) (•) measured experimental u_u, (o) u_u from measured $\overline{\rho u''c''}$, (▪) measured experimental u_b, (□) u_b from measured $\overline{\rho u''c''}$. **(J. Moss, 1980 [13])**

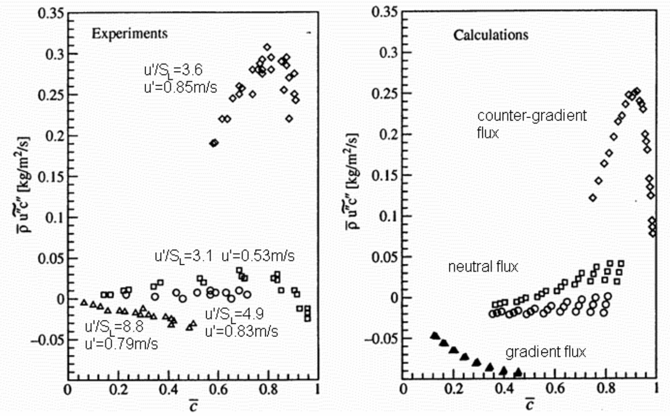


Fig.14 Comparison of calculated progress variable radial flux with experimental data from [39] **J. Frank, P. Kalt, R. Bilger, 1999 [14]**

Paradox 4: Chemistry dependence of the turbulent flame speed, which is observed in experiments at strong turbulence.

Question: How to explain this dependence keeping in mind

1.Quite plausible reasoning of the founders of the theory (G. Damkohler[15], K.Shchelkin [16], Ja.Zel'dovich) that at strong turbulence $u' >> S_L$ the flame speed does not depend on chemistry and can be estimated as $U_t \sim u'$;

2. Theoretical and experimental data on the speed of the front of turbulent diffusion which is close to the r.m.s. u' [17] and the speed of the front edge of the flame at $u' >> S_L$ is very closed to the speed of the diffusion front, and it give more accurate (than previous) theoretical estimation $U_t \cong u'$.

3.Resent DNS of the one-dimensional stationary flame at $u'/S_L = 4.8$, show that the speed of approach flow was close to u' (Hasegawa, T.,Himeno, R.,[18])

Explanation: Chemistry dependence in real flames is connected with the fact that they have increasing brush width. For transient flames the consumption speed and the speed of the front edge are different. While for the steady state flame the speed of the front edge controls the consumption rate, for the transient flame we must additionally to the flamelet speed U_f estimate the flamelet sheet area $(\bar{A}/A_0)$. It was done using some general properties of random surfaces and ideas of small scale equilibrium only for the case of thickened flamelet: $(\bar{A}/A_0) \sim Da^{3/4}$.

It results in [1], [2] $U_t \approx u' \cdot Da^{1/4} \approx u'^{3/4} \chi^{-1/4} S_L^{1/2} L^{1/4}$ (theoretical expression).

Conclusions

In the context of the analysed paradigm there are three stages of the flame:

1.Initial stage $0 < t < \tau_t$ when both small-scale and large-scale wrinkles are statistically nonequilibrium. The flame speed and width increases. $U_t \sim t,\quad \delta_t \sim t$ (It seems that this stage is actually significant only for SI engines.)

2.Intermediate stage $\tau_t < t < \tau_t \cdot Da$ when small-scale wrinkles are quasi-equilibrium and large-scale wrinkles are not equilibrium. In this case the width increases in accordance with the diffusion law $\delta_t \approx (D_t t)^{1/2}$ and at the same time the flame speed is nearly constant with $U_t \approx u' \cdot Da^{1/4} \approx u'^{3/4} L^{1/4} \chi^{-1/4} S_L^{1/2}$. This "intermediate steady propagation flames" are common in real burners.

3. In the final stage $t >> \tau_t \cdot Da$ the flame is steady state with $U_t \approx u'$. Such flames are practically unattainable as at real turbulence and chemistry flames crosses or reach walls (combustion is completed) long before the final stage.

In the second part of the presentation we present a joint RANS/LES approach to modeling premixed combustion, which is based on the ideas of small-scale equilibrium and gasdynamical nature of the counter-gradient transport effect.

Joint RANS/LES modelling of the premixed flames

We present an original timesaving joint RANS/LES approach to simulate turbulent premixed combustion. It is destined mainly for industrial applications where RANS approach is not sufficient, but complete replacing of it by LES practically impossible. It was proposed in [19], preprinted in [20], extended version is publishing in [21].

<u>The main peculiarities of the joint RANS/LES approach:</u>

1. RANS simulations predicts average fields, while following LES modeling gives an instantaneous image (potentialities for SI: RANS gives the mean indicator diagram, while LES can predicts cycle variations; for gas turbine applications: coupled with acoustic codes LES sub-problem can be used for analysis of unsteady combustion).
2. The main problem (agreement between RANS and averaged LES predictions) is accomplished by using the same principle of combustion modeling in RANS and LES sub-problems: as the combustion rate is controlled by unresolved small-scale coupling of turbulence and chemistry (“the challenge of turbulent combustion”) we assumed statistical small-scale equilibrium not only of Kolmogorov eddies, but also structures of reaction zones, and hence expressed theoretically RANS and LES flame speeds in terms of integral and subgrid turbulent parameters, and a chemical time, which is an integral characteristic of the chemical kinetics.
3. Mean dissipation rate from RANS simulations was used for estimation of the subgrid turbulence in the context of the Kolmogorov theory of small-scale turbulence (instead of the Smagorinsky model of subgrid turbulence) and in this case there are no subgrid viscosity fluctuations and it makes LES numerics more friendly.
4. RANS simulations need modeling large-scale turbulence, counter-gradient scalar flux, transient character of the real flame, while in LES give all these phenomena without modeling. Luckily, the RANS sub-problem can be formulated using only the gradient turbulent diffusion component of the flux with succeeding estimation of the counter-gradient pressure driven component of the flux at the post-processor stage.

Main equations

RANS sub-problem:

Actual flux — Actual source

$$\frac{\partial(\bar{\rho}\tilde{c})}{\partial t}+\nabla\cdot(\bar{\rho}\tilde{\vec{u}}\tilde{c})=-\nabla\cdot(\bar{\rho}\,\widetilde{\vec{u}''c''})+\bar{\rho}\tilde{W}$$

Unclosed equation

Turbulent diffusion gradient component — Gasdynamic counter-gradient component

$$\frac{\partial(\bar{\rho}\tilde{c})}{\partial t}+\nabla\cdot(\bar{\rho}\tilde{\vec{u}}\tilde{c})=\nabla\cdot(\bar{\rho}D_t\nabla\tilde{c})+\rho_u U_t|\nabla\tilde{c}|$$

Model flux — Model source

TFC model equation

Counter-gradient phenomenon has a gasdynamic (non turbulent) nature: different acceleration of reactant and product by the pressure gradient

$$\overline{\rho\vec{u}''c''}=\bar{\rho}(\bar{\vec{u}}_u-\bar{\vec{u}}_b)\tilde{c}(1-\tilde{c})=\underbrace{-\bar{\rho}D_t\nabla\tilde{c}}_{\text{Turbulence}}+\underbrace{(\bar{\rho}(\Delta\bar{\vec{u}}_{p-d})\tilde{c}(1-\tilde{c}))}_{\text{Gasdynamics}},$$

The $"k-\varepsilon"$ model is applicable even when the scalar flux is counter- as the gasdynamic component is estimated on the post-process stage

$$U_t=Au'Da^{1/4}=Au'^{3/4}L^{1/4}S_L^{1/2}\chi^{-1/4},\quad A\approx 0.5$$

Theoretical expression (from small-scale equilibrium)

LES sub-problem

$$\frac{\partial(\bar{\rho}_\Delta\tilde{c}_\Delta)}{\partial t}+\nabla\cdot(\bar{\rho}_\Delta\tilde{\vec{u}}_\Delta\tilde{c}_\Delta)=\nabla\cdot(\bar{\rho}_\Delta D_\Delta\nabla\tilde{c}_\Delta)+\rho_u U_t^\Delta|\nabla\tilde{c}_\Delta|$$

Model equation

$$U_t^\Delta=A^\bullet u_\Delta'^{3/4}S_L^{1/2}\chi^{-1/4}\Delta^{1/4},\quad A^\bullet\approx 1.2$$

Subgrid flame speed (theoretical expression)

The Kolmogorov’s subgrid turbulence (theoretical expressions)

$$E(k)=C\varepsilon^{2/3}k^{-5/3}$$ **inertial spectrum**

$$u_\Delta'^2\approx\int_{1/\Delta}^{\infty}E(k)dk\approx\varepsilon^{2/3}\Delta^{2/3}$$ **subgrid turbulent energy**

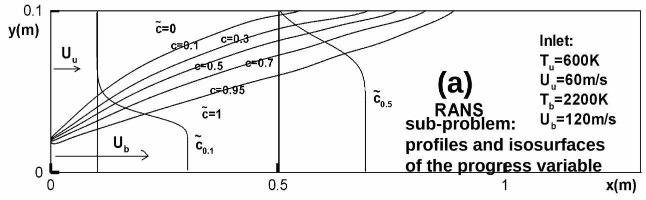
$$L_\Delta\approx\int_{1/\Delta}^{\infty}k^{-1}E(k)dk\Big/\int_{1/\Delta}^{\infty}E(k)dk\approx\Delta$$ **subgrid scale of turbulence**

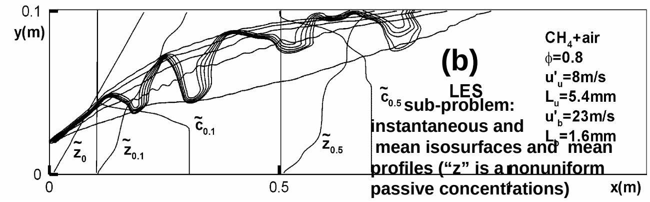
$$D_\Delta\approx\nu_\Delta\approx u_\Delta'L_\Delta\approx\varepsilon^{1/3}\Delta^{4/3}$$ **subgrid turbulent diffusion and viscosity coefficients**

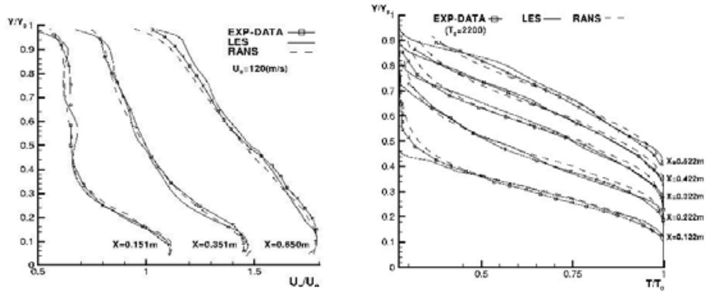
In LES the mean dissipation rate ε is taken from RANS simulations.

Joint RAMS/LES examples (simulations were performed by V. Battglia, “Fluent”):

I. ONERA (Moreau) standard burner [22]



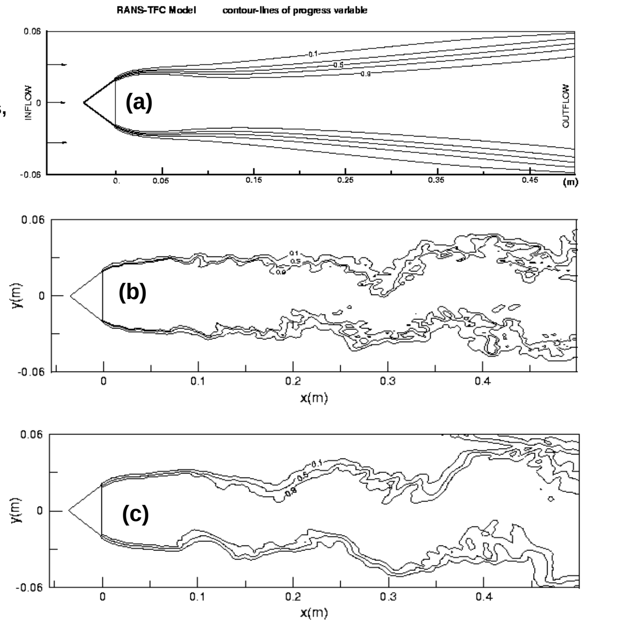




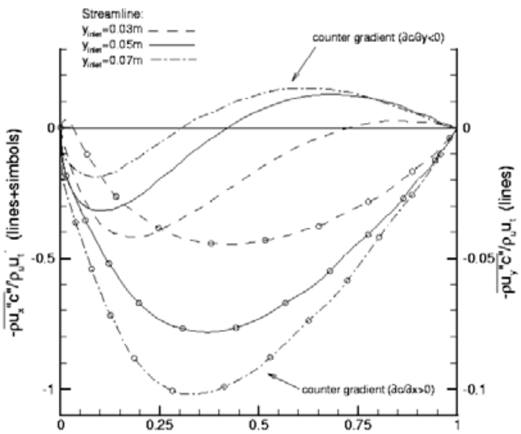
Comparison of RANS and average LES profiles with the experimental data

II. Volvo flame (triangular bluff body, rectangular channel) [23]

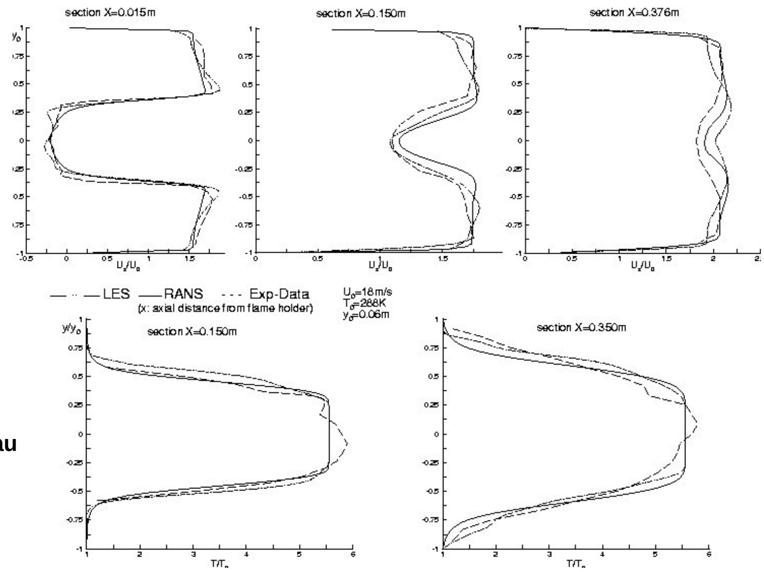
C3H8-air,
F=0.65,
Uo =18m/s,
u' =3%,
To=288K.



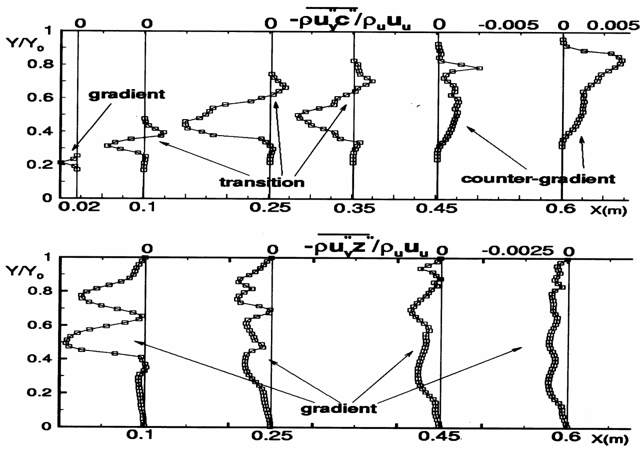
(a)RANS sub-problem;
(b) joint LES sub-problem, Kolmogorov subgrid turbulence;
(c) LES with the Smagorinsky turbulence [24] (for comparison).



RANS longitudinal and lateral scalar flux (RANS *modeling* predicts strong counter-gradient flux for longitudinal and transition from gradient to counter-gradient flux for lateral component in the Moreau burner with high velocities and strong turbulence

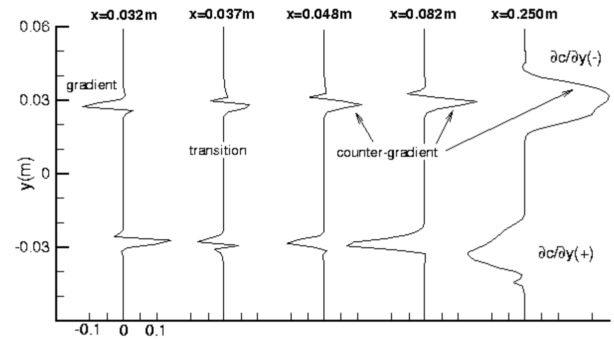


Comparison of RANS and average LES profiles with the VOLVO data



LES simulation (*without modeling*) of the mean lateral scalar flux of progress variable “c” (transition from gradient to counter-gradient flux along the flame) and nonuniform passive addition “z” (a gradient flux everywhere), i.e. *at the same point we can have counter-gradient (reacting species) and gradient (passive species) fluxes*

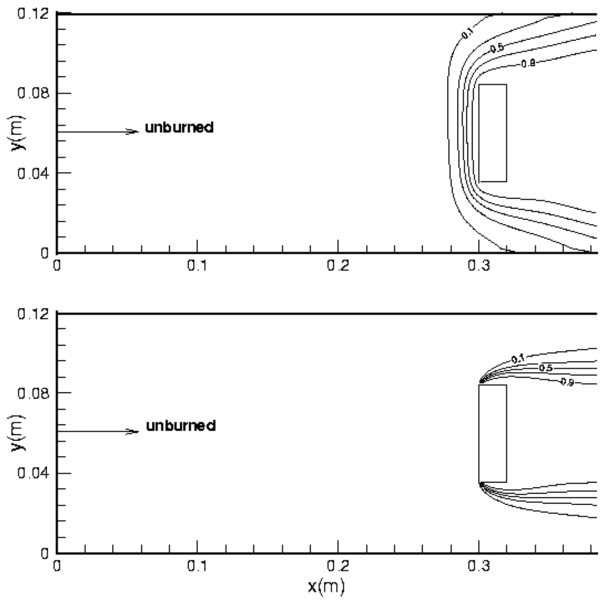
Paradox 1: positive and negative diffusion in the same point



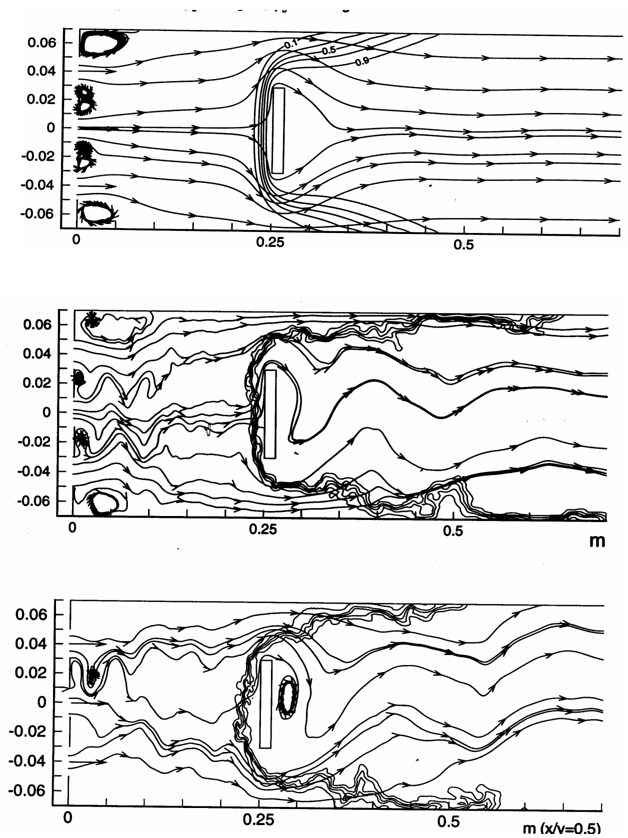
Averaged LES lateral scalar flux: we see transition from the gradient to the counter-gradient scalar flux in the flame with continuously increasing brush width.

Paradox 2: the brush width grows in spite of negative diffusion

III. The impinging flame, joint RANS/LES approach



Two configurations of the flame (RANS sub-problem)

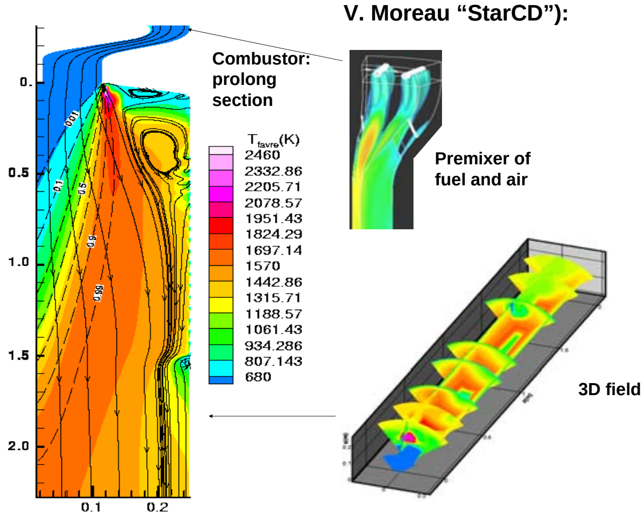


RANS and two instantaneous images of LES (without initial data for turbulence)

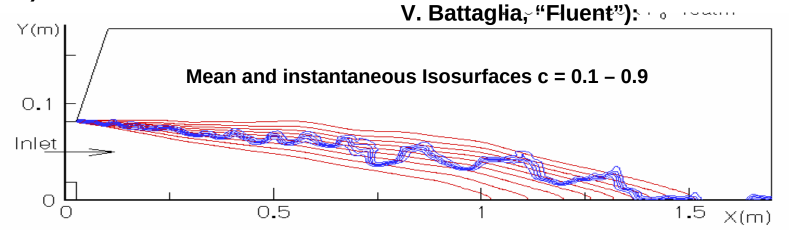
IV. 3D RANS/LES simulation of the GE10 combustor [25]

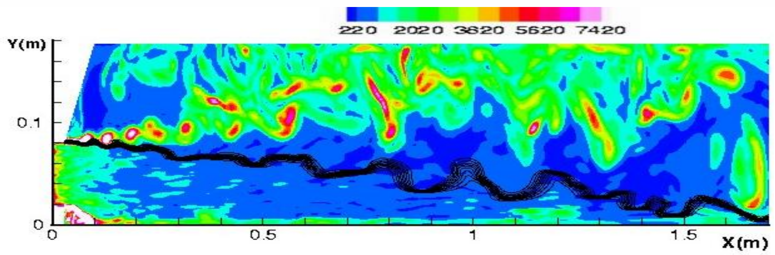
Inlet conditions:
U_{in}=80 m/s, Turb. intensity=10% Φ=0.49 T_{in}=660K, P_0=15atm

RANS sub-problem (simulations were performed by V. Moreau "StarCD"):

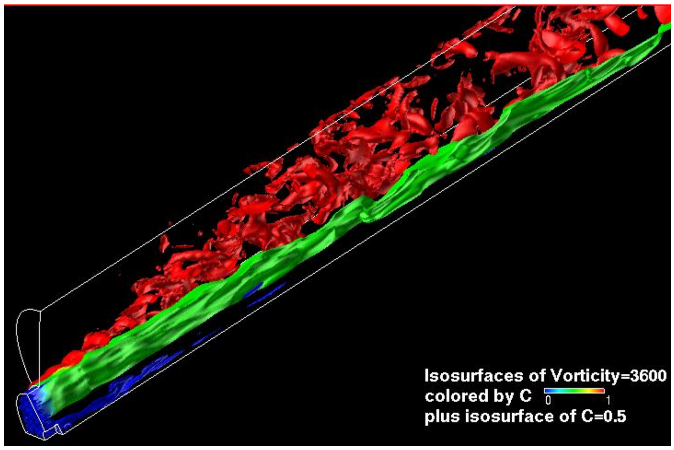


LES sub-problem (simulations were performed by V. Battaglia, "Fluent"):





LES instantaneous vorticity magnitude field (2D section) with the contour-lines of the progress variable C = 0.1 - 0.9 ΔC=0.2



Conclusions:

1. We developed the joint RANS/LES approach, validated it and applied to real gas turbine.
2. From a numerical viewpoint our LES sub-problem is more friendly and les time consuming in comparison with traditional LES as the grid size and time step can be relatively large.
3. We see next applications to gas turbines and SI engines:
   a. Coupling LES sub-problem with an acoustic code to testing of a RANS result for combustion instability;
   b. To analyze cycle-to-cycle variations corresponding to a RANS simulation.

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